Designability of nanostructures for thermal transport

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Expanding the limits of low and high thermal conductivity of solid materials or realizing the current state-or-art values with other more abundant or multifunctional materials is the key challenge in thermal engineering (management, harvest, and reuse). To this end, recent progresses in material fabrication and characterization at the nanoscale has brought great advance in thermal science to understand the correlation between the lattice heat conduction of semiconductors and insulators and their atomistic structures. With this, now the demand for predicting and designing optimal materials is higher than ever. In order to overcome the vast parameter space of exploration, it is natural to consider combining thermal science and data science for high throughput screening and optimization of compounds and structures. In this talk, we will introduce some of our recent researches to (1) find crystalline compounds with high or low thermal conductivity by hierarchical screening, and (2) design nano/interfacial structures by coupling phonon transport calculation and optimization method. In (1), the route from the large database of crystal (compound) structures to the small database of thermal conductivity is divide into several steps with database sizes that gradually shrinks. Screening is then performed on each link between the steps differently accounting for the size of the database to enhance the screening efficiency and accuracy. In (2), we developed a framework by alternating between thermal-transport calculations and informatics-based optimization technique. The results so far demonstrate the effectiveness and advantage of materials informatics in predicting/designing structures for phonon transport, which can be extended to other transport properties.